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INTRODUCTION

In the discrete ordinates, or S_N, numerical solution of the transport equation, both the spatial ($\underline{r}$) and angular ($\underline{\Omega}$) dependences on the angular flux $\psi(\underline{r},\underline{\Omega})$ are modeled discretely. Significant effort has been devoted toward improving the spatial discretization of the angular flux [1, 2]. In this work, we focus on improving the angular discretization of $\psi(\underline{r},\underline{\Omega})$. In the conventional S_N method, the angular dependence is modeled with a quadrature of discrete angles. Instead, we employ a Petrov-Galerkin quadratic finite element approximation for the differencing of the angular variable (μ) in developing the one-dimensional (1D) spherical geometry S_N equations. We develop an algorithm that shows faster convergence with angular resolution than conventional S_N algorithms.

SPHERICAL TRANSPORT EQUATION

This 1D spherical transport equation in conservative form is given by

$$\begin{aligned}&\frac{\mu}{r^2}\frac{\partial}{\partial r}\left[r^2\psi(r,\mu)\right]+\frac{1}{r}\frac{\partial}{\partial \mu}\left[(1-\mu^2)\psi(r,\mu)\right]\\&+\Sigma(r)\psi(r,\mu)=S(r,\mu).\end{aligned} \tag{1}$$

We discretize the angular variable with a set of N angular bins, with boundaries $\mu_1<\mu_2<\ldots<\mu_n<\ldots<\mu_{N+1}$, and $\mu_1=-1$. $\mu_1=-1$ is the starting direction and is treated separately from the other directions. [3, 4] The angular flux for the direction μ_n is $\psi(r,\mu_n)=\psi_n$. (The spatial dependence is omitted.)

Conventional Methods

The standard formulation of the S_N equations involves the diamond-difference (DD) relationship between the angular fluxes for angle n and “half-angles” $n-1/2$ and $n+1/2$:

$$\psi_{n+1/2}=2\psi_n-\psi_{n-1/2}. \tag{2}$$

To preserve the solution of a uniform isotropic flux in an infinite medium ($\psi(r,\mu) = S/\Sigma$) for any quadrature set, differencing coefficients $\alpha_{n+1/2}$ are used in the angular derivative term to force the two streaming terms to vanish. [3, 4] Upon spatial differencing, we obtain the conventional S_N equations. In addition, Morel and Montry have developed a "weighted diamond-difference" algorithm that is more accurate than standard DD. [5]

DESCRIPTION OF THE ACTUAL WORK

Our new method employs Petrov-Galerkin finite elements for $\psi(r,\mu)$ in Eq. (1). Specifically, we approximate the angular dependence as a combination of a continuous piecewise bilinear function and a continuous quadratic function of μ :

$$\psi(r,\mu) \cong \psi_n\left(\frac{\mu_{n+1}-\mu}{\Delta\mu_n}\right) + \psi_{n+1}\left(\frac{\mu-\mu_n}{\Delta\mu_n}\right) + \tilde{\psi}_n\left[\frac{4(\mu_{n+1}-\mu)(\mu-\mu_n)}{\Delta\mu_n^2}\right], \quad (3)$$

where $\mu_n \le \mu \le \mu_{n+1}$ and $\Delta\mu_n = \mu_{n+1} - \mu_n$. (Eq. (3) is valid in the first angular bin $-1 < \mu \le \mu_2$.) To obtain the discrete equations, Eq. (3) is substituted for $\psi(r,\mu)$ in Eq. (1), and then we operate on Eq. (1) by $\int_{\mu_n}^{\mu_{n+1}} (\cdot) d\mu$ in each angular bin; that is, $1 \le n \le N$. The result is the following:

$$\begin{aligned}&\frac{\Delta\mu_n}{6r^2}\frac{d}{dr}\{r^2[\psi_n A(\mu) + \psi_{n+1}B(\mu) + 2\tilde{\psi}_n C(\mu)]\} + \frac{1}{r}[\psi_{n+1}(1-\mu_{n+1}^2) - \psi_n(1-\mu_n^2)] + \\ &\frac{\Sigma(r)\Delta\mu_n}{2}[\psi_n + \psi_{n+1} + \frac{4}{3}\tilde{\psi}_n] = S(r)\Delta\mu_n,\end{aligned} \quad (4)$$

where $A(\mu) = \mu_{n+1} + 2\mu_n$, $B(\mu) = 2\mu_{n+1} + \mu_n$, and $C(\mu) = \mu_{n+1} + \mu_n$. This equation has one known angular flux (ψ_n) and two unknown angular fluxes (ψ_{n+1} and $\tilde{\psi}_n$). Thus, we need another equation. That equation is obtained by substituting Eq. (3) for $\psi(r,\mu)$ in Eq. (1), and then operating on Eq. (1) by $\int_{\mu_n}^{\mu_{n+1}} (\cdot)\mu d\mu$. The result is

$$\begin{aligned}&\frac{\Delta\mu_n}{12r^2}\frac{d}{dr}\{r^2[\psi_n D(\mu) + \psi_{n+1}E(\mu) + \frac{4}{5}\tilde{\psi}_n F(\mu)]\} + \frac{1}{r}\{\psi_{n+1}[\mu_{n+1}(1-\mu_{n+1}^2) - \frac{\Delta\mu_n}{2} + \frac{\Delta\mu_n}{12}E(\mu)] - \\ &\psi_n[\mu_n(1-\mu_n^2) + \frac{\Delta\mu_n}{2} - \frac{\Delta\mu_n}{12}D(\mu)] - \tilde{\psi}_n[\frac{2\Delta\mu_n}{3} - \frac{\Delta\mu_n}{15}F(\mu)]\} + \frac{\Sigma(r)\Delta\mu_n}{6}[\psi_n A(\mu) + \psi_{n+1}B(\mu) \\ &+ 2\tilde{\psi}_n C(\mu)] = \frac{S(r)(\mu_{n+1}^2 - \mu_n^2)}{2},\end{aligned} \quad (5)$$

where $D(\mu) = \mu_{n+1}^2 + 2\mu_{n+1}\mu_n + 3\mu_n^2$, $E(\mu) = 3\mu_{n+1}^2 + 2\mu_{n+1}\mu_n + \mu_n^2$, and $F(\mu) = 3\mu_{n+1}^2 + 4\mu_{n+1}\mu_n + 3\mu_n^2$.

Upon spatial differencing Eqs. (4) and (5), we have the discretized equations for our quadratic finite element method. These equations are solved similarly to the conventional S_N equations by marching through the grid in the direction of particle motion. To obtain the starting value at $\mu = -1$, we do a separate calculation for the first angular bin boundary at $\mu = -1$, similarly to what is done in conventional S_N methods. [3, 4] This gives us the values for ψ_1 in each radial zone. This equation resembles a planar geometry transport equation. Next, using Eqs. (4) and (5), we determine the fluxes in every radial zone for the remaining angular bin boundaries starting with μ_2 and ending with μ_{N+1}. For the incoming directions, $\mu_n < 0$, we march inward from the outer boundary to the center of the sphere. Then, for the outgoing directions, $\mu_n > 0$, we march outward from the center to the sphere boundary. However, in this new method, two unknown fluxes exist (ψ_{n+1} and $\tilde{\psi}_n$); thus, we must solve a system of equations given by Eqs. (4) and (5) for each radial zone.

RESULTS

To demonstrate the strength of the QFE method, we consider several test problems. The first problem, proposed by Lathrop [4], is a simple two region sphere. The inner region contains a uniformly distributed isotropic source with a small total cross section. The outer region material has a total cross section that is five times larger without any source. The media in both regions are pure absorbers, so this problem neglects scattering. Also, this problem does not contain energy dependence.

For several different quadrature sets, we determine the absorption and leakage rates for both the weighted DD and our new quadratic finite element (QFE) schemes. The results indicate the QFE method converges much faster than the weighted DD scheme with finer angular resolution. For example, the leakage rate from the QFE scheme is within 0.3% of the exact solution when using four angles. However, the leakage rate from the weighted DD scheme is an enormous 49% below the analytical solution when using four angles. Even for 32 angles, the leakage rate from weighted DD remains 1.7% below the exact solution. For QFE, the leakage rate is highly converged with just eight angles.

Because the number of unknowns for QFE is twice the number of unknowns for weighted DD, the cost of QFE is double the cost of weighted DD for a given number of angles. Thus, to be equitable, QFE with N angles should be compared to weighted DD with 2N angles. For example, the leakage rate from QFE is within 0.03% of the exact solution for eight angles, while weighted DD is within 6% of the exact solution for 16 angles. Overall, the results indicate that QFE with N angles is more closely converged to the exact solution than weighted DD with 2N angles.

The second problem is a modification of the Planet Critical Sphere (Pu-Met-Fast-018). This problem contains an inner sphere of plutonium surrounded by a layer of beryllium. To study supercritical systems, we increase the beryllium thickness. To model this, energy dependence, fission sources, and anisotropic scattering (P_2) are included. Using both DD and QFE, we determine the **α** eigenvalue for several different quadrature sets. In DD, the **α** converges to within 0.1 μsec^{-1} after increasing the number of angles beyond 32. For QFE, the **α** converges to within 0.1 μsec^{-1} after the number of angles exceeds 8. Thus, for DD to achieve the same level of accuracy as QFE, DD requires four times as many angles as QFE.

We plan to present results from at least two additional problems.

In summary, we have developed a new higher-order S_N algorithm for the solution of the 1D spherical transport equation using quadratic finite elements. This method shows excellent convergence with relatively coarse angular resolution. This convergence rate has been shown to be superior to conventional S_N techniques for 1D spherical geometry. In the future, we plan to study and compare the QFE algorithm with Lathrop's new Quadratic Continuous method [4]. The goal will be to understand why the QFE method shows better convergence rates. Also, we hope to extend the ideas of QFE to higher dimensions and to different geometries. (U)

REFERENCES

1. J.E. MOREL, T.A. WAREING, and K. SMITH, "A Linear-Discontinuous Spatial Differencing Scheme for S_N Radiative Transfer Calculations," *J. Comput. Phys.*, **128**, 445 (1996).
2. A. GREENBAUM and J.M. FERGUSON, "A Petrov-Galerkin Finite Element Method for Solving the Neutron Transport Equation," *J. Comput. Phys.*, **64**, 97 (1986).
3. E.E. LEWIS and W.F. MILLER, JR., *Computational Methods of Neutron Transport*, 135-145, American Nuclear Society, Inc., La Grange Park, Illinois (1993).
4. K.D. LATHROP, "A Comparison of Angular Difference Schemes for One-Dimensional Spherical Geometry S_N Equations," *Nucl. Sci. Eng.*, **134**, 239 (2000).
5. J.E. MOREL and G.R. MONTRY, "Analysis and Elimination of the Discrete-Ordinates Flux Dip," *Transp. Theory Stat. Phys.*, **13**, 615 (1984).

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